

Amendments to the Specification

1. Please delete the title and add the following new title:
A Method of Analysing Chemical Data and a Computer Program Product for the Same
2. Please replace the paragraph that begins with “This metric can be performed” at page 3, line 15, with the following amended paragraph:

This metric can be performed in a single pass through the data; therefore it requires comparatively few processing steps and does not require memory for storage of intermediate results. Specifically, to calculate the metric, squared Euclidian distances are calculated between points in a matrix of N points by N points and each point and the co-ordinate centre; a vector of N points[[]]. The memory required for each additional vector is $1/N^{\text{th}}$ of memory required for distance matrix and therefore insignificant. Moreover, the number of calculations required for additional vector is $1/N^{\text{th}}$ of calculations required for distance matrix. Having calculated these distance matrix and vector it is possible in one pass apply two thresholds:

- Threshold for squared Euclidian distance; and
- Threshold for the metric of the invention.

3. Please replace the paragraph that begins with “The embodiment of the invention processes” at page 4, line 24, with the following amended paragraph:

The embodiment of the invention processes a multi-dimensional set of data that is generated from the results of multiple chemical analyses, for example, ~~from~~ from a quantitative structure-activity relationship (QSAR) or a quantitative structure-property (QSPR) programme. The chemical analyses are performed using conventional analysts apparatus and methods and the results are stored in a machine-readable file. The file is then read by analysis software executing on a computer to generate an analysis output that can be interpreted by a person or be passed to another computer system or computer program for further analysis.

4. Please replace the paragraph at page 4, line 19, that immediately follows the heading “Brief Description of the Drawing”, with the following amended paragraph:

~~Figure 1~~ The figure is a block diagram of an analysis embodying the invention.

5. Please replace the paragraph that begins with “In the analysis, the data” at page 5, line 11, with the following amended paragraph:

In the analysis, the data is subject to five principle processing steps, as will now be described. These steps and the data that they produce and operate upon are shown in ~~Figure 1~~ the accompanying drawing.